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Anomalous electrical resistivity and Hall constant of Anderson lattice with finite f-band width

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Abstract : We study here an extension of the periodic Anderson model by considering finite f-band width. A variational method is used to study the temperature dependence of electronic transport properties of Anderson lattice for different values of the f-band width. The electrical resistivity $\rho(T)$ and Hall constant $R_H(T)$ calculated show qualitatively the features experimentally observed in heavy fermion materials. We find that as f-band width increases, the low temperature peak in $\rho(T)$ disappears, while the low-temperature peak in $R_H(T)$ becomes sharper.

Keywords : Anderson lattice, electrical resistivity, Hall constant

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1. Introduction

Anomalous transport properties are characteristic features of mixed valence (MV) and heavy fermion (HF) compounds [1]. The experimental results of electrical resistivity $\rho(T)$ of many heavy fermion systems (e.g. $CeAl_3$, $CeCu_2Si_2$, $CeCu_6$, UBe_{13}) at low temperatures show anomalous behaviour [2-6]. $\rho(T)$ increases with increasing temperature in the very low temperature region, reaching a maximum and then decreases slowly like lnT at higher temperatures.

The Hall constant $R_H(T)$ also exhibits characteristic anomalies when compared to the Hall constant of usual metals. The Hall constant in heavy fermion Ce compounds *e.g.* $CeAl_3$, $CeCu_2Si_2$, $CeCu_6$, $CeRu_4Si_2$ is much larger than in normal metals, often positive and generally drops rapidly at low temperature [7, 8]. The mechanism for this is skew scattering, arising from strong spin orbit coupling for the f-impurity. A theoretical model of the skew scattering by Kondo impurities of Cerium was first proposed in the early seventies [9]. This model treats the skew scattering by using the Coqblin-Schrieffer interaction [10] and is valid only well above the Kondo temperature (T_k). More recently, Coleman, Anderson and Ramakrishnan [11, 12] (CAR) have presented a calculation which describes the skew scattering by Cerium impurities in both limits $T >> T_k$ and $T << T_k$. The single-impurity models of Fert [9] and CAR [11, 12] are strictly valid only in the incoherent regime where the heavy fermion systems can be pictured as a collection of independent resonant scattering centers. At present, there is no specific theory of the skew scattering in the presence of coherence effects. However, some features of the experimental results at low temperatures can be accounted for by extrapolating the single-impurity results into the coherent regime [11, 12].

In the recent past, the periodic Anderson model (PAM) has been widely accepted as a model for understanding the basic electronic and magnetic properties of MV and HF materials. In fact, there is an overlap of 5 f orbital (thereby giving rise to a finite f-band width) in actinide materials [13]. We consider here

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an extension of the PAM by considering finite f-band width. Recently an extension to the Anderson model in which direct f–f hopping is included has been studied by many authors [14-17]. This model has been studied by several authors using the variational method [18-20].

We developed recently, a variational method [21-25] to study the ground state thermodynamic properties of PAM. We use this variational method here to study the PAM including finite f-band width. In Section 2, we give the basic formulation for electrical resistivity and Hall constant. In Section 3, we discuss our results

2. Basic formulation

The orbitally nondegenerate periodic Anderson model including finite band width of f-electrons is described by the Hamiltonian

$$H=\sum_{k\sigma}\epsilon_k C^{+}_{k\sigma}C_{k\sigma}+\sum_{ij\sigma}T_{ij}b^{+}_{i\sigma}b_{j\sigma}$$

$$-\sum_{ik\sigma}V_{ik}\left(c^{+}_{k\sigma}b_{i\sigma}+h.c.\right)+\frac{U}{2}\sum_{i\sigma}n^{f}_{i\sigma}n^{f}_{i-\sigma}\,, \tag{1}$$

where $$T_{ij}=\frac{1}{N}\sum_{k}E_k e^{ik(R_i-R_j)} \tag{2}$$

Here, E_k is the f-band energy and other symbols have their usual meanings.

For simplicity, we assume that the form of the f-band is the same as that of the conduction band The f-band is represented by the expression

$$E_k=\epsilon_f+A\left|\epsilon_k-\frac{W}{2}\right|, \tag{3}$$

where A is a positive constant less than unity. Here, W and AW are the band widths of conduction band and f-band, respectively. For $A=0$, $E_k=\epsilon_f$ is the position of the f-level.

In k-space, Anderson Hamiltonian may be written as

$$H=\sum_{k\sigma}\epsilon_k c^{+}_{k\sigma}c_{k\sigma}+\sum_{k\sigma}\left[\epsilon_f+A\left(\epsilon_k-\frac{W}{2}\right)\right]b^{+}_{k\sigma}b_{k\sigma}$$

$$-\sum_{k\sigma}V_k\left(c^{+}_{k\sigma}b_{k\sigma}+h.c.\right)+\frac{U}{2}\sum_{i\sigma}n^{f}_{i\sigma}n^{f}_{i} \tag{4}$$

Here, we are considering strongly interacting (*i.e.* $U\to\infty$) case. In this case, the probability of f^2 configuration is very small. The variational wave function which projects f^2 configuration out, may be written as [21].

$$|\psi\rangle=\prod_{k\sigma}\left[1+A_{k\sigma}(1-n^{f}_{-\sigma})b^{+}_{k\sigma}c_{k\sigma}\right]|F\rangle. \tag{5}$$

where $|F\rangle=\prod_{k\le k_{F\sigma}}c^{+}_{k\sigma}|0\rangle$

is the Fermi sea of conduction electrons and $A_{k\sigma}$ are variational parameters.

With this wave function, the variational parameter and the number of conduction and f-electrons at finite temperatures are respectively, given by

$$A_{k\sigma}=\frac{1}{2V_kP_f^2}\Big[\epsilon_k(1-AP_f)-\epsilon_fP_f+\frac{AWP_f}{2}$$

$$+\sqrt{\left|\epsilon_k(1-AP_f)-\epsilon_fP_f+\frac{AWP_f}{2}\right|^2+4V_k^2P_f^2}\Big]$$

where $P_f=\left(1-n^{f}_{-\sigma}\right)$.

$$n^{c}_{\sigma}=\frac{1}{N}\sum_{k}\frac{f_{k\sigma}}{1+A^{2}_{k\sigma}P_f^2}$$

$$n^{f}_{\sigma}=\frac{1}{N}\sum_{k}\frac{A^{2}_{k\sigma}P_f^2f^{-}_{k\sigma}}{1+A^{2}_{k\sigma}P_f^2}$$

where $f^{-}_{k\sigma}=f\left(E^{-}_{k\sigma}-\mu\right)$ is the Fermi function for the lower branch of the quasi-particle spectrum. The expression $E^{-}_{k\sigma}$ is given by

$$E^{-}_{k\sigma}=\frac{1}{2}\Big[\left(1+AP_f\right)\epsilon_k+\epsilon_fP_f-\frac{AWP_f}{2}$$

$$-\sqrt{\left|\left(1-AP_f\right)\epsilon_k-\epsilon_fP_f+\frac{AWP_f}{2}\right|^2+4V_k^2P_f^2}\Big] \tag{9}$$

Let $N^{c}_{\sigma}(\epsilon_k)$ denote the density of the unperturbed conduction band, $N^{t}(E^{-}_{k\sigma})$ the total density of the lower quasi-particle states, $N^{c}(E^{-}_{k\sigma})$ the density of the (lower part of the) perturbed conduction states. Then

$$N^{c}(E^{-}_{k\sigma})=N^{t}(E^{-}_{k})n^{c}_{k\sigma}=\frac{N^{t}(E^{-}_{k})}{1+A^{2}_{k\sigma}P_f^2}, \tag{10}$$

$$N^{t}(E^{-}_{k\sigma})=\frac{N^{c}(\epsilon_k)}{\left(dE^{-}_{k\sigma}/d\epsilon_k\right)},$$

where

$$\frac{d E_{k\sigma}^{-}}{d \in_k} = \frac{-E_{k\sigma}^{-} + (1 - AP_f)\left[AP_f \in_k + \in_f P_f - \frac{AWP_f}{2}\right]}{\left[\left[\in_k (1 - AP_f) - \in_f P_f + (AWP_f / 2\right]^2 + 4v_k^2 p_f^2\right]^{1/2}} \quad (12)$$

A Electrical resistivity :

We are not interested here in the absolute value of resistivity, but only in the variation of resistivity with temperature. We use the electrical conductivity formula given by Mott and also used by us in Ref. [23]

$$\sigma(T) = \int \left(\frac{-\partial f_{k\sigma}}{\partial \in_{k\sigma}^{-}}\right) \tilde{\sigma}\left(E_{k\sigma}\right) d\ E_{k\sigma}^{-}, \quad (13)$$

where $\tilde{\sigma}\left(E_{k\sigma}\right)$ can be written as

$$\tilde{\sigma}\left(E_{\sigma}^{-}\right) = \sigma_0 \left[N'\left(E_{k\sigma}^{-}\right)\right]^2 \quad (14)$$

with $$\sigma_0 = \frac{2\pi e^2 \hbar^3}{m^2} |D_k \quad av \quad (15)$$

B Hall constant .

The Hall constant $R_H(T)$ due to skew scattering is given by the expression

$$R_H(T) = \sigma \bar{\chi}(T) \rho(T), \quad (16)$$

where $\bar{\chi}(T)$ is the normalized magnetic susceptibility $\chi(T)' = \chi(T)/C$ (C being the Curie constant) and $\rho(T)$ is the electrical resistivity. The coefficient γ takes on different values γ_1 and γ_2 above and below Kondo temperature T_K as discussed by Fert and Levy [8]. In this work we are only limited to simple model calculations of $R_H(T)$ of Heavy Fermion systems. However, for γ (*i.e.* for γ_1 and γ_2), we take values of $CeAl_3$ compound which is a prototype of a class of HF materials. For this compound, $\gamma_1 = 0.075\ K/T$ for $T>T_K$ and $\gamma_2 = 0.097\ K/T$ for $T<T_K$. $T_K = 40K$ [8].

In the presence of a static magnetic field B, the f-level is

$$\chi(T) = g\sigma\mu_B \frac{\partial}{\partial B}\left[n_{\sigma}^f - n_{-\sigma}^f\right]_{B \to 0} \quad (17)$$

Putting n_{σ}^f's from (8), one gets the expression of susceptibility for $U \to \infty$ [17] in units of $(g\mu_B)^2$.

3. Results and discussion

In these calculations, we have considered tight binding conduction band $\in_k = -\cos k$ with conduction band-width $W = 2.0$ eV. The total number of electrons per site $(n^c + n^f)$ has been taken to be 1.5. The f-band width is $AW=2A$. V is fixed on 0.25 eV. We have calculated the temperature dependence of electrical resistivity $\rho(T)$ and Hall constant for different values of parameter A and different effective positions of the f-level $\in_f$.

Figure 1(a) shows the variation of electrical resistivity $\rho(T)$ with temperature for different values of parameter A. ε_f is fixed on 0.0. In Figure 1(b), we show the $\rho(T)$ for different effective positions of f-level A is fixed on 0.15 and ε_f =0.0. In both the figures for finite value of A, we do not get rapid increase in $\rho(T)$ at low temperatures and the maxima at low temperature also disappears Further as we increase A. $\rho(T)$ increases in the whole temperature range. In Figure 1(b), as the f-level shifts downward with respect to Fermi energy ε_f, $\rho(T)$ increases more sharply in the low temperature regime. But we do not get any maxima at low temperature. It means the maxima at low temperature which disappears on the introduction of finite f-band width in the Anderson Hamiltonian, can not be reproduced by varying ε_f positions downward with respect to ε_f. However, our resistivity result for $A = 0.0$ and ε_f = -0.6, -0.4, -0.2 are in qualitative agreement with the experimental results of many heavy fermion materials like $YbAgCu_4$ and MV compounds like $CePd_3$ [23].

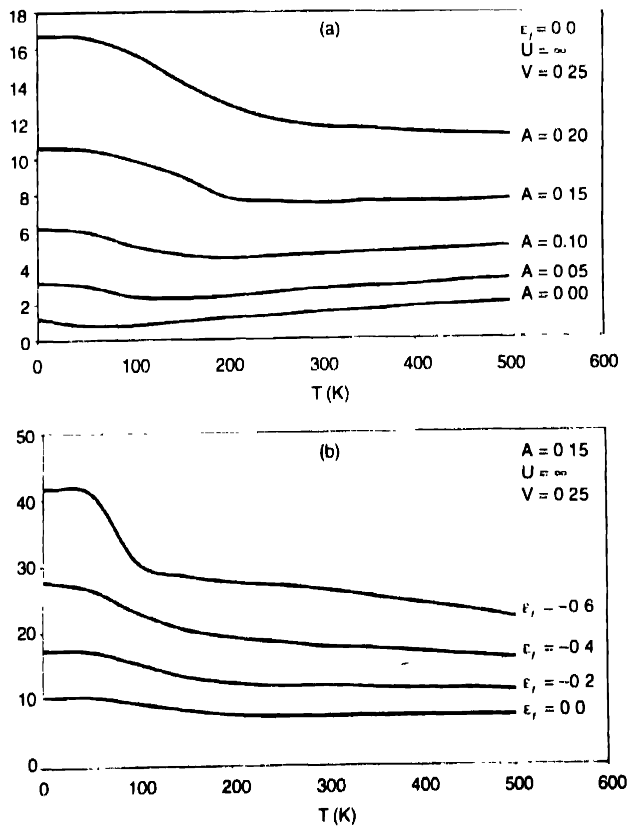

Figure 1. Variation of electrical resistivity $\rho(T)$ with temperature with tight-binding conduction band, V = 0.25, (a) for different values of A and (b) for different effective positions of f-level ε_f

Corresponding results for the temperature dependence of the Hall constant $R_H(T)$ for different values of A are shown in Figure 2. Figure 2 shows the typical behaviour in $R_H(T)$ with a rapid increase in $R_H(T) \sim T^2$ at low temperature, has a maxima at temperature 50 K and then $R_H(T)$ decreases towards higher temperature for all values of A. In all cases, $R_H(T)$ remains positive in the given temperature range which is the main characteristics of heavy fermion Cerium compounds like $CeAl_3$ [8].

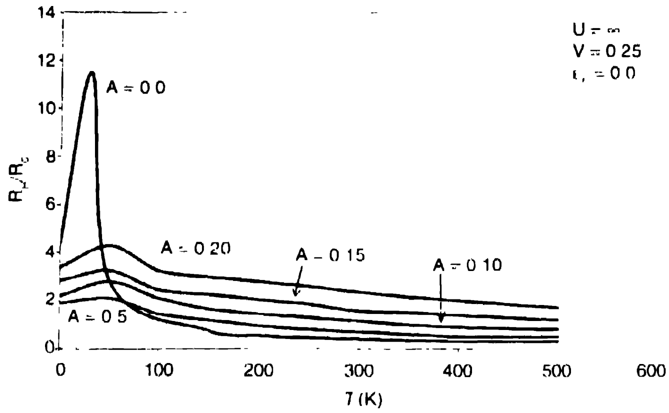

Figure 2. Hall constant $R_H(T)$ as a function of temperature with tight binding conduction band, for different values of A

Similar behaviour of $R_H(T)$ has been observed in other heavy fermion compounds like $CeCu_6$, $CeRu_2Si_2$, UPt_3 *etc*. We see further that as A is increased from 0.0, $R_H(T)$ increases with land remains positive. We do not see the change of sign at higher temperatures. However, we find the singular behaviour in $R_H(T)$ at low temperature below 50K for $A = 0.0$ where the maxima in $R_H(T)$ becomes more sharp and becomes more pronounced when compared with the maxima for finite A.

We expect large anomalous Hall constants to occur generally in the mixed valence and heavy fermion systems where the almost localised f-electrons form narrow quasi-particle bands, extremely sensitive to a magnetic field. At low temperatures, in very pure compounds, true heavy bands will be formed. In this regime, the current carried by each Bloch state will have a skew component differing widely between different Fermi- surface regions, so that the resultant Hall effect can be derived from a detailed band structure and transport theory. In near future, we plan to take into account these factors and calculate the Hall resistivity and Hall constant at low temperatures.

From the above results of $\rho(T)$ and $R_H(T)$, one can conclude that by increasing f-band width we are making the Fermi-liquid nature of f-electrons more pronounced.

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